Bridging the Gap Between Microscale Modeling and Additive Manufacturing for TPS

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AMA at Thermal Protection Materials Branch (ARC-TSM)

March 29th, 2022

Additively Manufactured Thermal Protection System (AMTPS) Workshop

Predictive Material Modeling (PMM) group

Entry System Modeling (ESM) project

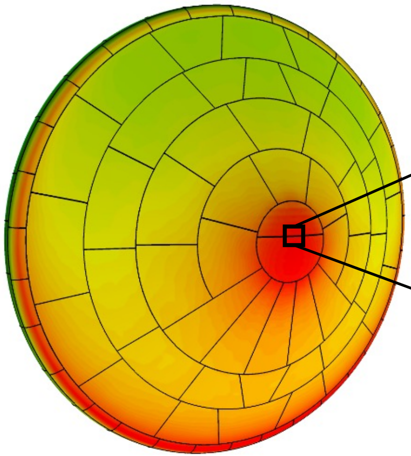
Content

- Motivation
- Overview of PuMA
  - Functionalities
  - Open-source release
  - Artificial generation
  - Micro-CT manipulation
- Effective properties for anisotropic porous media
  - Fiber orientation
  - Conductivity
  - Elasticity
  - Permeability
  - Real-time micro-CT

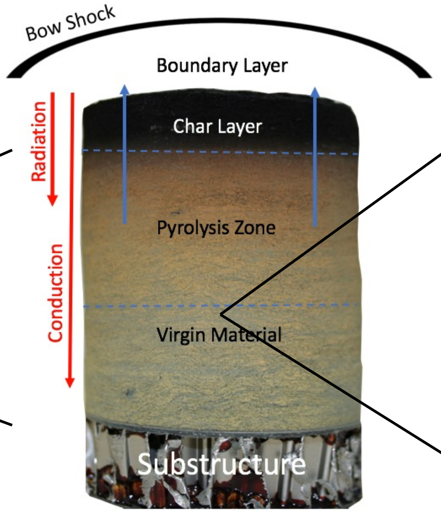
Modeling TPS

Macroscale

Full-scale material response solvers, using homogenized properties



Simulation of surface temperature for MSL heatshield

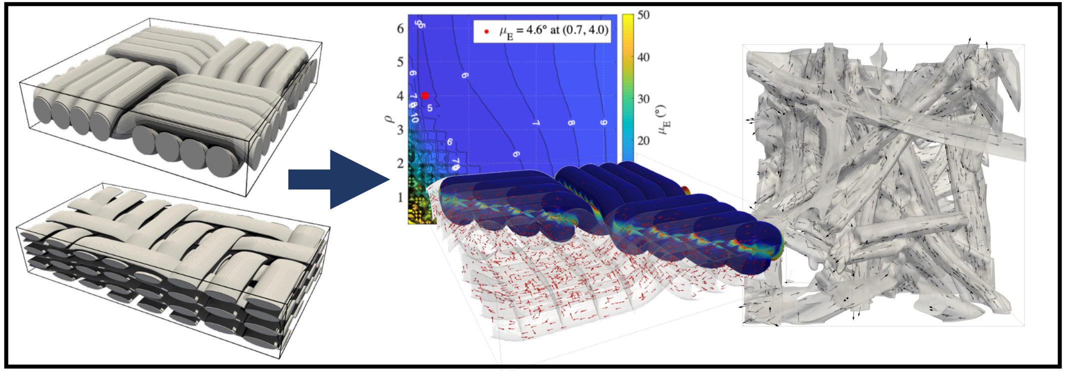


Microscale

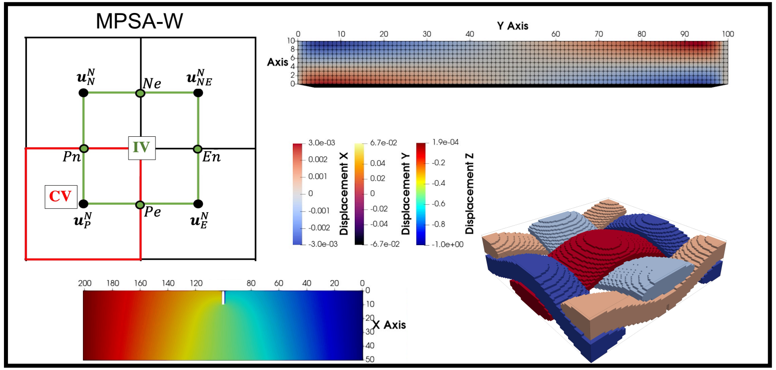
Homogenization of material properties to be used in macroscale models

Overview of material properties computation

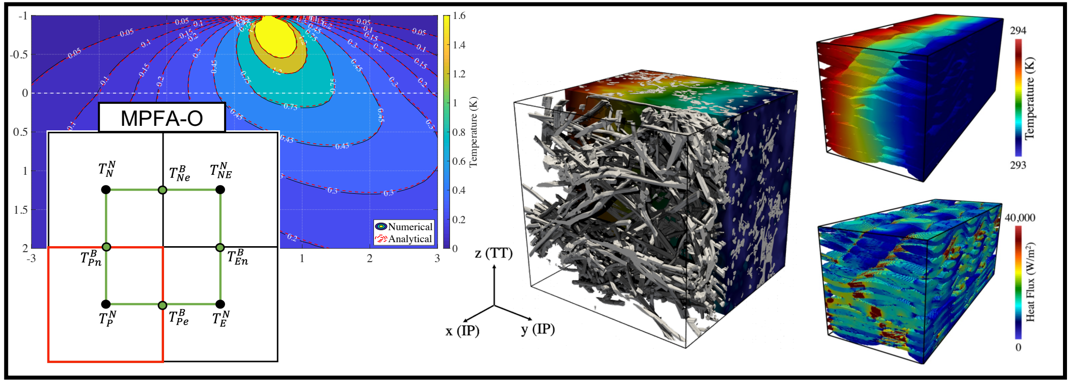
Part 1: Estimation of local orientation. *Computational Materials Science* (2020)



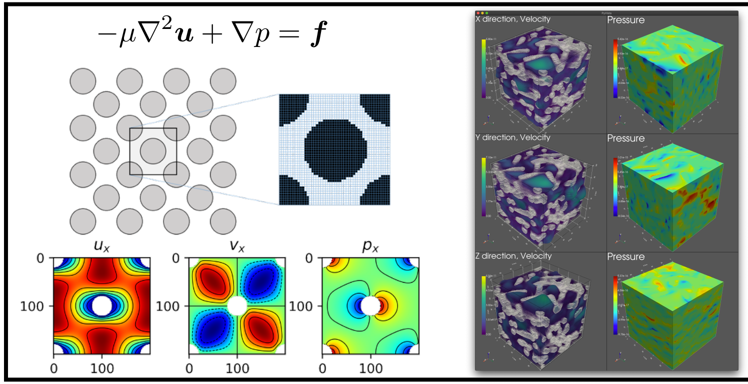
Computation of effective elasticity



Part 2: Computation of effective conductivity. *Computational Materials Science* (2021)



Computation of effective permeability



Porous Microstructure Analysis (PuMA) v3 release

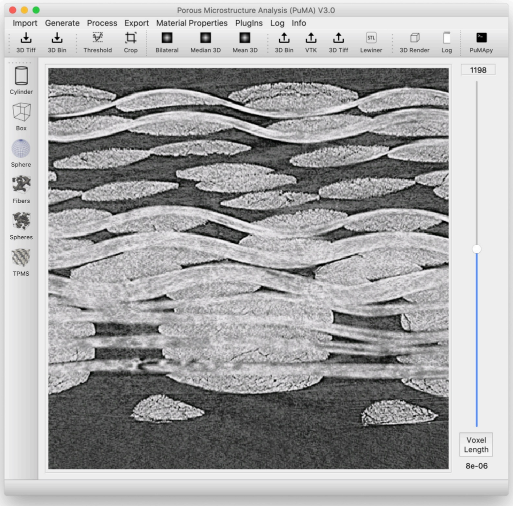
Installation: conda install -c conda-forge puma

Open-source repository: https://github.com/nasa/puma

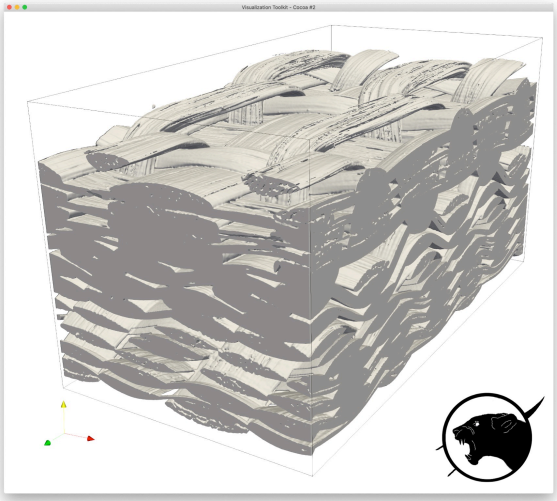
Documentation: https://puma-nasa.readthedocs.io

Video tutorials: PuMA YouTube channel

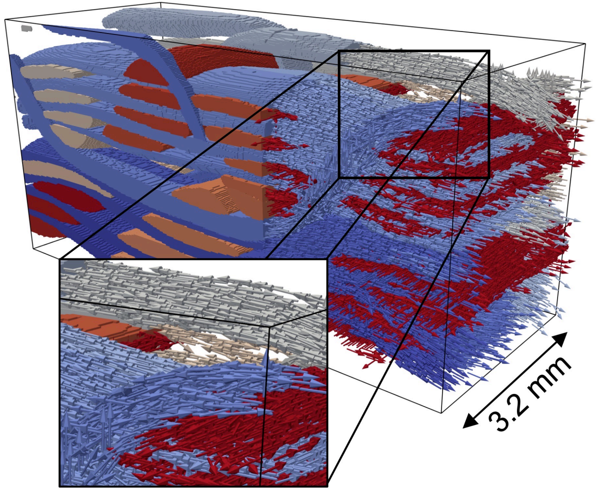
a)



b)



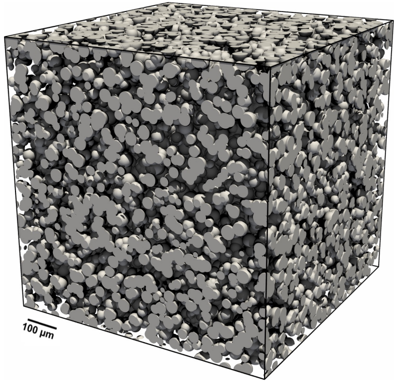
c)



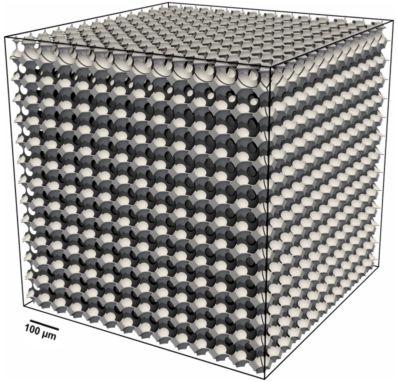
Ferguson, J.C., Semeraro, F., Thornton, J.M., Panerai, F., Borner, A., Mansour, N.N., 2021. Update 3.0 to “PuMA: The Porous Microstructure Analysis software”, *SoftwareX*

Artificial domain generation

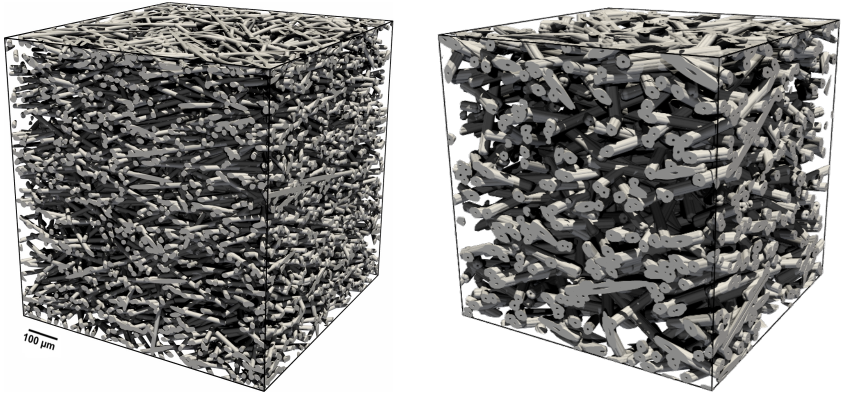
Packed Sphere Beds



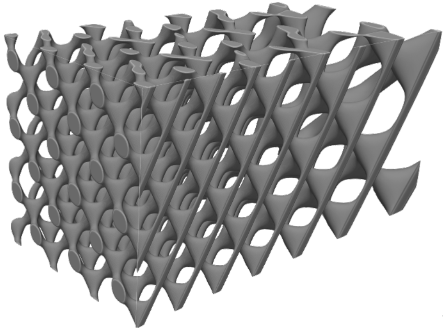
Periodic Foams



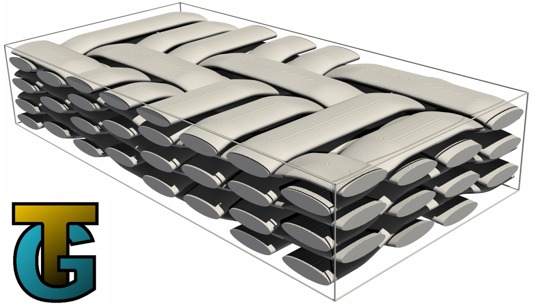
Fiber Structures



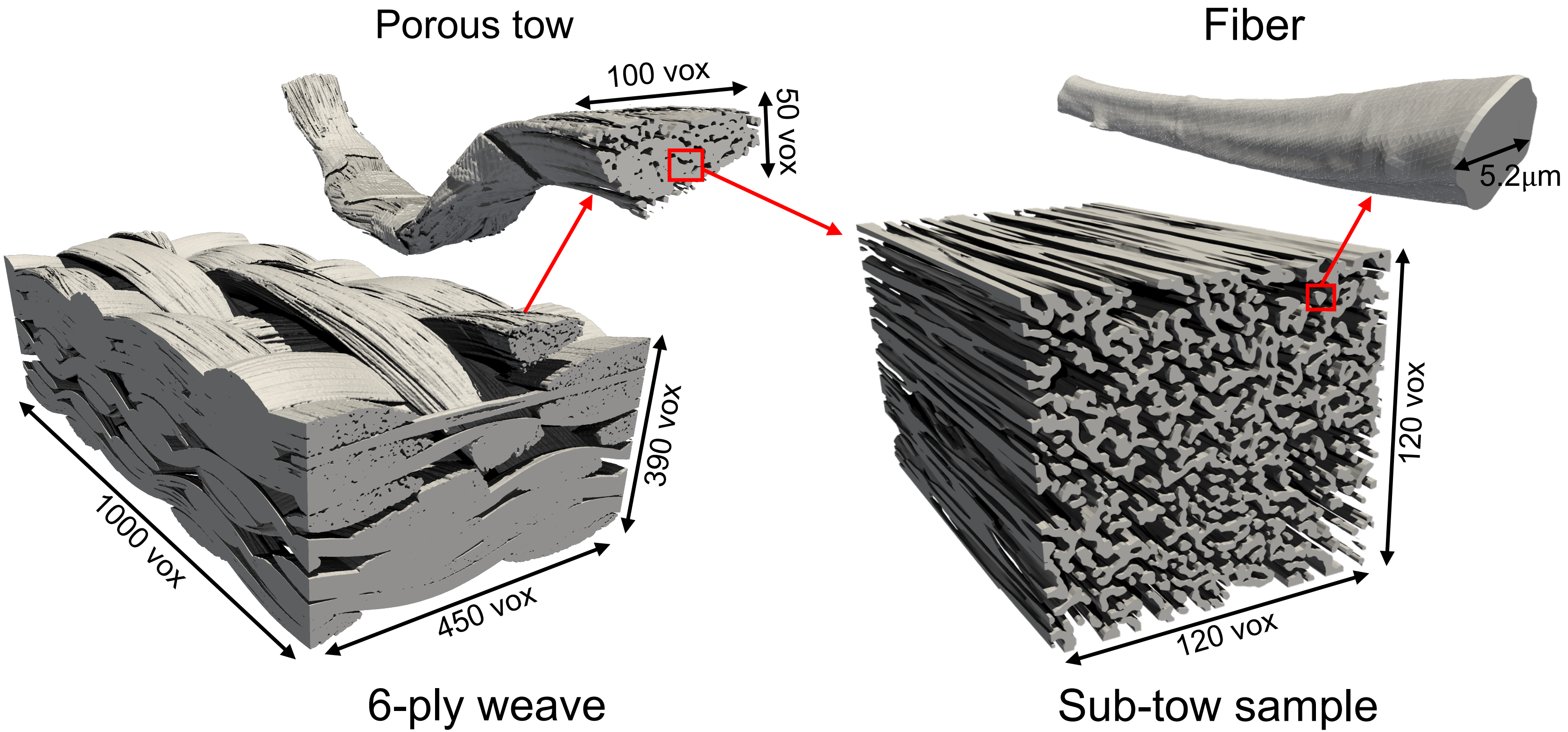
Triply Periodic Minimal Surface (TPMS)



Woven geometries

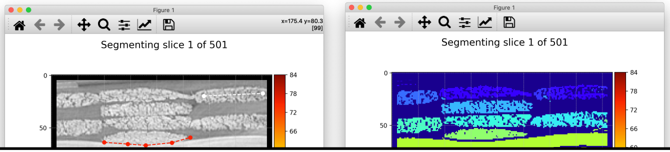


Micro-CT weaves: anisotropic at multiple scales

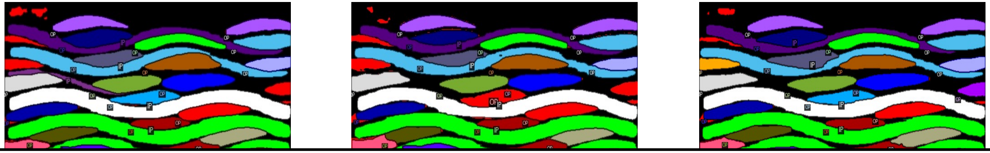


Weave segmentation and tow tracking

Manual labeling

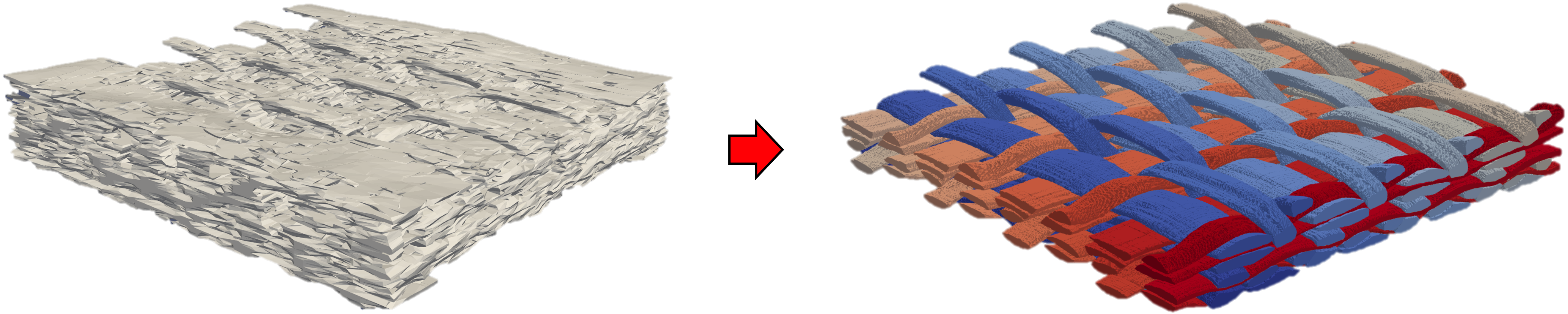


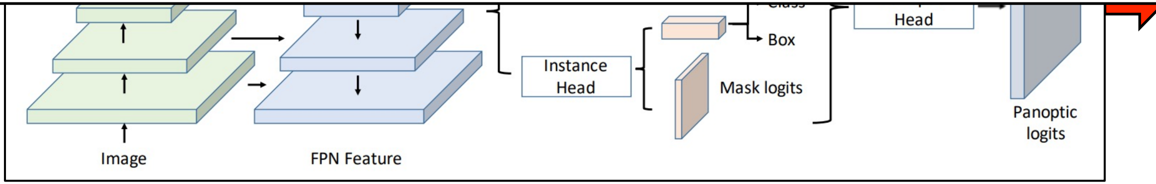
Tracking by IoU

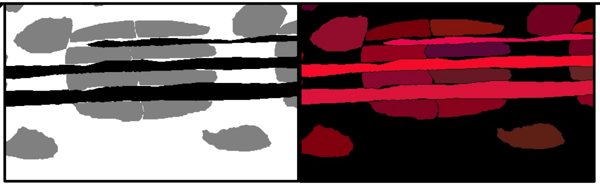


Naïve threshold of original Micro-CT weave

Fully segmented weave







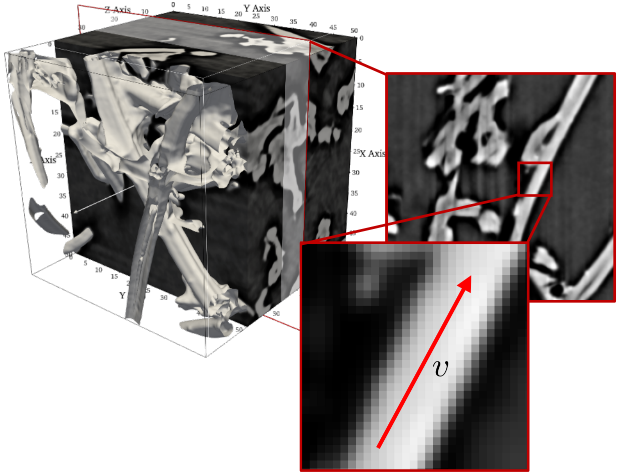
Semantic Classes

Instances

Allred, A., Abbott, L.J., Doostan, A., Maute, K. Automated processing of x-ray computed tomography images via panoptic segmentation for modeling woven composite textiles, *Composite Structures* (accepted)

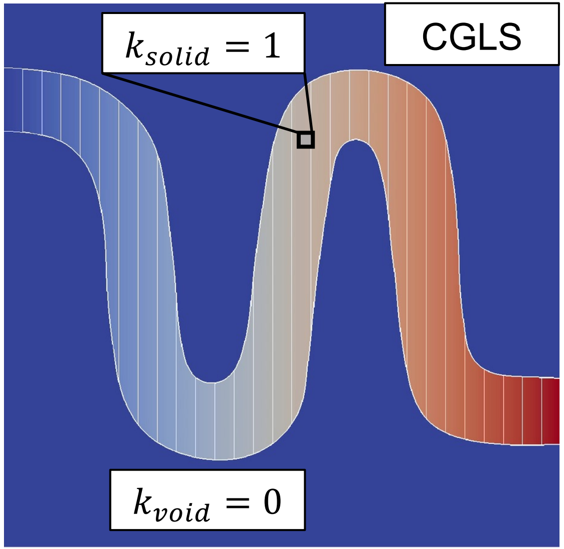
Orientation methods

Structure tensor

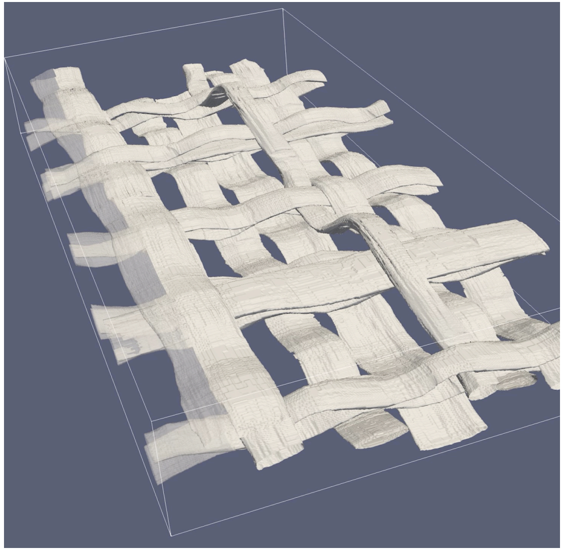


$$(I(x+v) - I(x))^2 \approx 0$$

Artificial flux



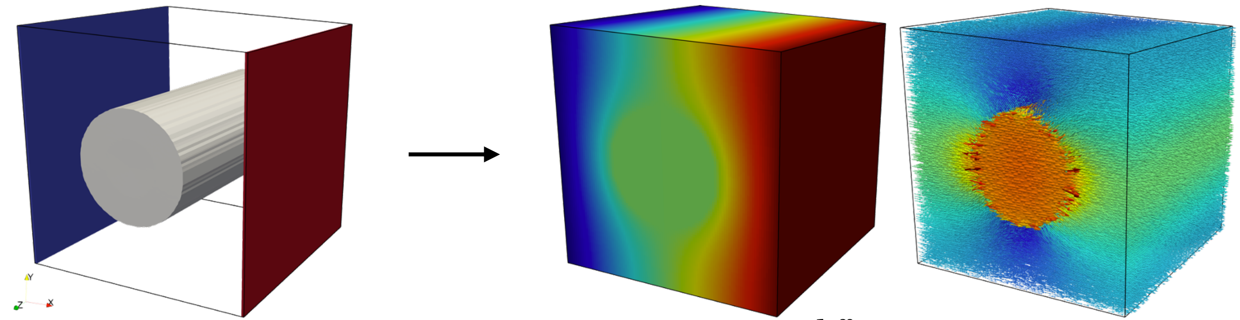
Ray casting



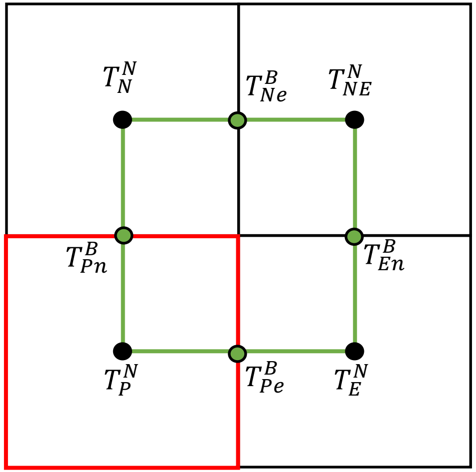
Semeraro, F., Ferguson, J.C., Panerai, F., King, R.J. and Mansour, N.N., 2020. Anisotropic analysis of fibrous and woven materials part 1: Estimation of local orientation. *Computational Materials Science*, *178*, p.109631.

Conductivity solver

$$\nabla \cdot \boldsymbol{q} = 0 \quad \text{where} \quad \boldsymbol{q} = -\boldsymbol{k}\nabla T = -\begin{bmatrix} k^{xx} & k^{xy} & k^{xz} \\ k^{xy} & k^{yy} & k^{yz} \\ k^{xz} & k^{yz} & k^{zz} \end{bmatrix} \begin{pmatrix} \partial T/\partial x \\ \partial T/\partial y \\ \partial T/\partial z \end{pmatrix}$$



$$\boldsymbol{k}^x = -\boldsymbol{q} \cdot L_x$$



Multi-Point Flux Approximation (MPFA-O)* local system (2D):

$$\boldsymbol{q} = \boldsymbol{E}\boldsymbol{T}^N$$

$$\boxed{q_P^x} = k_P^{xx}\frac{T_{Pe}^B - T_P^N}{h/2} + k_P^{xy}\frac{T_{Pn}^B - T_P^N}{h/2}$$

Unknowns:

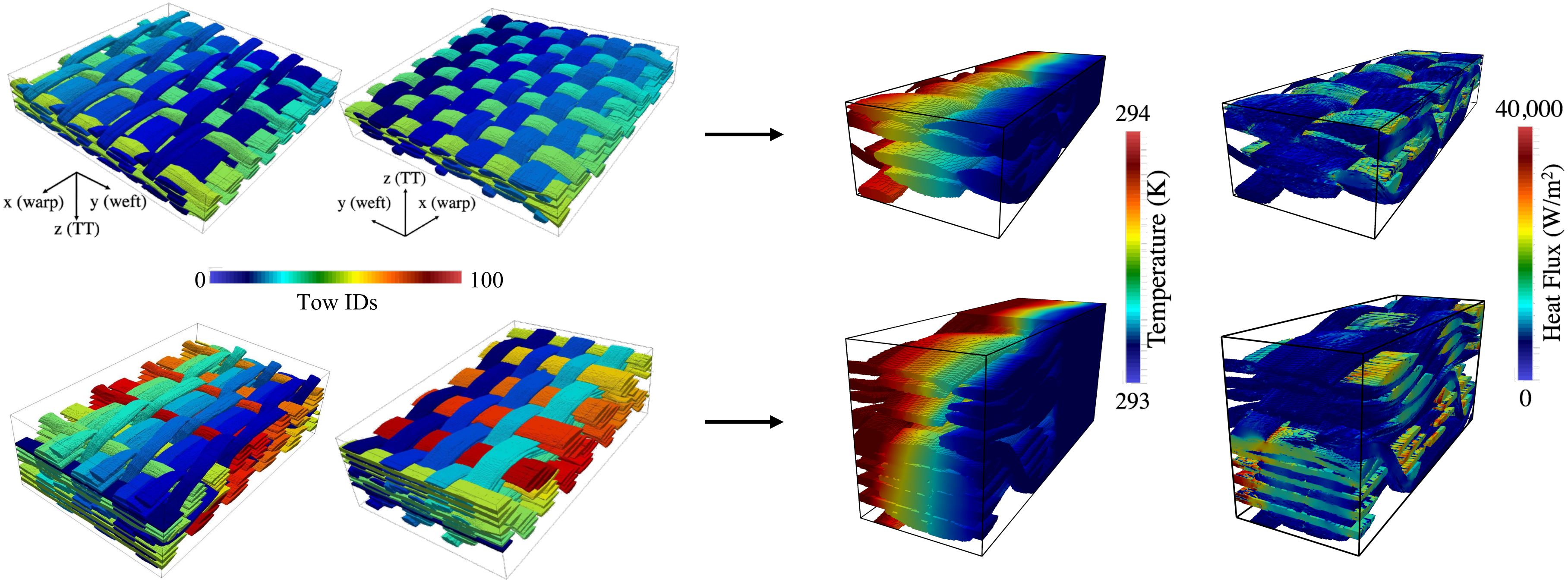
$$\boldsymbol{T}^B = \begin{pmatrix} T_{Pe}^B \\ T_{Ne}^B \\ T_{Pn}^B \\ T_{En}^B \end{pmatrix}$$

Continuity of fluxes:

$$\boxed{q_P^x} = q_E^x$$
$$q_N^x = q_{NE}^x$$
$$q_P^y = q_N^y$$
$$q_E^y = q_{NE}^y$$

*Ivar Aavatsmark. Multipoint flux approximation methods for quadrilateral grids. *9th International forum on reservoir simulation 2007*, *Abu Dhabi*, pages 9–13.

Conductivity solver validation: ADEPT

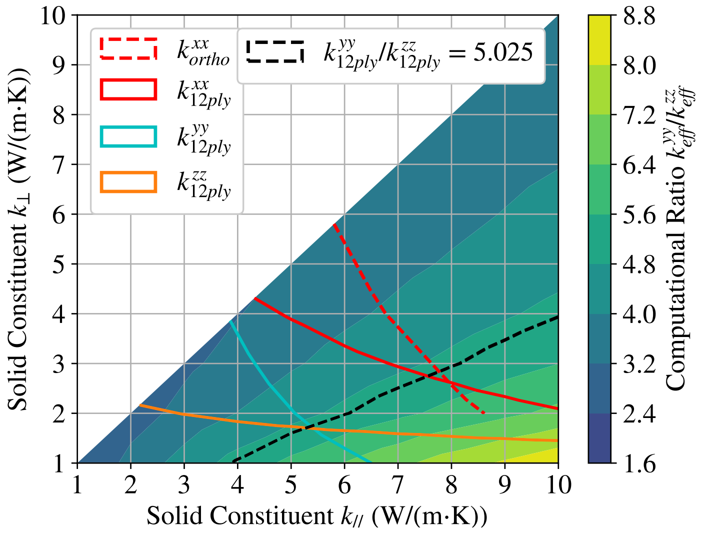


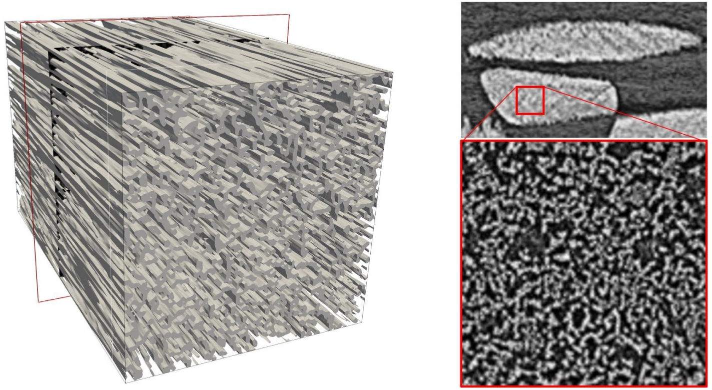
Semeraro, F., Ferguson, J.C., Acin, M., Panerai, F. and Mansour, N.N., 2021. Anisotropic analysis of fibrous and woven materials part 2: Computation of effective conductivity. Computational Materials Science, 186, p.109956.

Single fiber conductivity estimation

Experimental value at room temperature:

$$\boldsymbol{k}_{exp}^{12ply} = \begin{bmatrix} 2.184 & - & - \\ - & 1.980 & - \\ - & - & 0.394 \end{bmatrix}$$





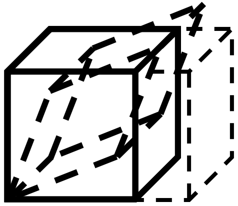
Single fiber thermal conductivity

$$[k_{//}, k_{\perp}] = [9.7, 5.5]\frac{\mathrm{W}}{\mathrm{mK}}$$

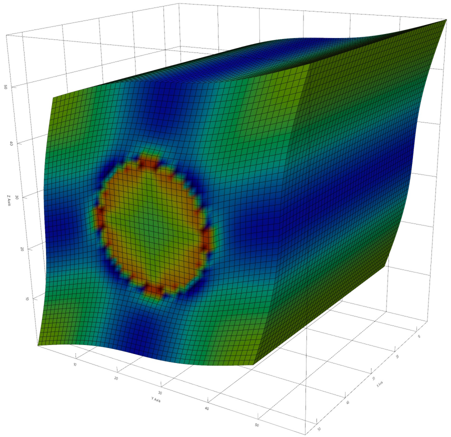
$$\boldsymbol{k}_{num}^{12ply} = \begin{bmatrix} 2.310 & -0.414 & 0.000 \\ -0.524 & 2.030 & 0.071 \\ 0.007 & 0.050 & 0.504 \end{bmatrix}$$

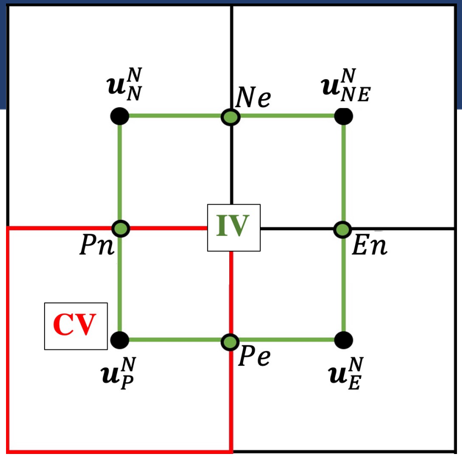
Elasticity solver

$$\nabla \cdot \boldsymbol{\sigma} = 0 \quad \text{where} \quad \boldsymbol{\sigma} = \boldsymbol{C}\boldsymbol{\varepsilon}$$



$$\boldsymbol{C}^4 = \frac{2L_xL_y}{L_x + L_y}\boldsymbol{\sigma}$$





Continuity of Stresses and Displacements:

$$\begin{aligned}
\boxed{\boldsymbol{\sigma}_P^{xx}} &= \boldsymbol{\sigma}_E^{xx} & u_P^x + u_P^{xx}/2 &= u_E^x - u_E^{xx}/2 \\
\boldsymbol{\tau}_P^{yx} &= \boldsymbol{\tau}_E^{yx} & u_P^y + u_P^{yx}/2 &= u_E^y - u_E^{yx}/2 \\
\boldsymbol{\sigma}_N^{xx} &= \boldsymbol{\sigma}_{NE}^{xx} & u_N^x + u_N^{xx}/2 &= u_{NE}^x - u_{NE}^{xx}/2 \\
\boldsymbol{\tau}_N^{yx} &= \boldsymbol{\tau}_{NE}^{yx} & u_N^y + u_N^{yx}/2 &= u_{NE}^y - u_{NE}^{yx}/2 \\
\boldsymbol{\sigma}_P^{y} &= \boldsymbol{\sigma}_N^{yy} & u_P^x + u_P^{xy}/2 &= u_N^x - u_N^{xy}/2 \\
\boldsymbol{\tau}_P^{xy} &= \boldsymbol{\tau}_N^{xy} & u_P^y + u_P^{yy}/2 &= u_N^y - u_N^{yy}/2 \\
\boldsymbol{\sigma}_E^{yy} &= \boldsymbol{\sigma}_{NE}^{yy} & u_E^x + u_E^{xy}/2 &= u_{NE}^x - u_{NE}^{xy}/2 \\
\boldsymbol{\tau}_E^{xy} &= \boldsymbol{\tau}_{NE}^{xy} & u_E^y + u_E^{yy}/2 &= u_{NE}^y - u_{NE}^{yy}/2
\end{aligned}$$

Multi-Point Stress Approximation (MPSA-W)* local system (2D):

$$\boldsymbol{\sigma} = \boldsymbol{E}\boldsymbol{u}^N$$

$$\boxed{\boldsymbol{\sigma}_P} = \boldsymbol{C}_P\boldsymbol{G}_P - \langle \boldsymbol{C}\tilde{\boldsymbol{Q}}\boldsymbol{G}\rangle_{IV}$$

$$\begin{pmatrix} \boldsymbol{S}_G \\ \boldsymbol{D}_G \end{pmatrix} \boldsymbol{G} = \begin{pmatrix} \boldsymbol{0} \\ \boldsymbol{D}_u \end{pmatrix} \boldsymbol{u}^N + \begin{pmatrix} \boldsymbol{F}_N \\ \boldsymbol{D}_d \end{pmatrix}$$

Unknowns:

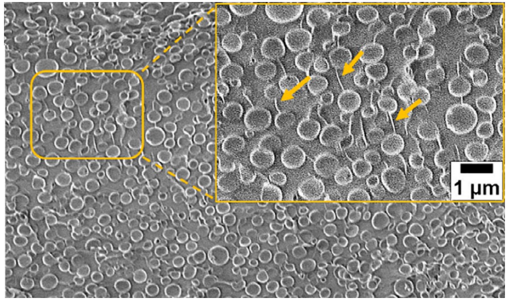
$$\boldsymbol{G} = \begin{pmatrix} \boldsymbol{G}_P \\ \boldsymbol{G}_E \\ \boldsymbol{G}_N \\ \boldsymbol{G}_{NE} \end{pmatrix} \qquad \boldsymbol{G}_P = \begin{pmatrix} u_P^{xx} \\ u_P^{yy} \\ u_P^{xy} \\ u_P^{yx} \end{pmatrix}$$

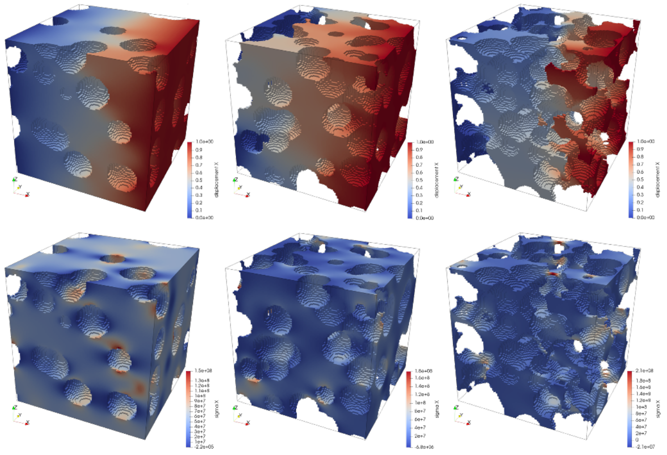
*Keilegavlen, E. and Nordbotten, J.M., 2017. Finite volume methods for elasticity with weak symmetry. Int. Journal for Numerical Methods in Engineering, 112(8), pp.939-962.

Elasticity solver validation: woven composite

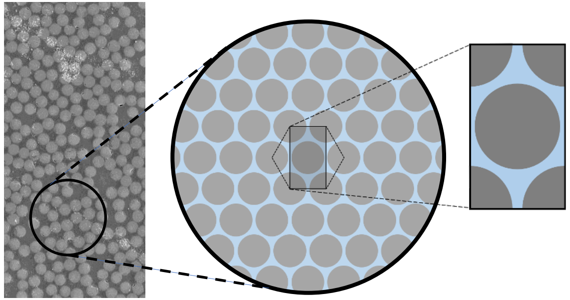
Fraile Izquierdo, S., Semeraro, F., Acin, M., 2022. Multi-Scale Analysis of Effective Mechanical Properties of Porous 3D Woven Composite Materials. *AIAA Scitech Forum*

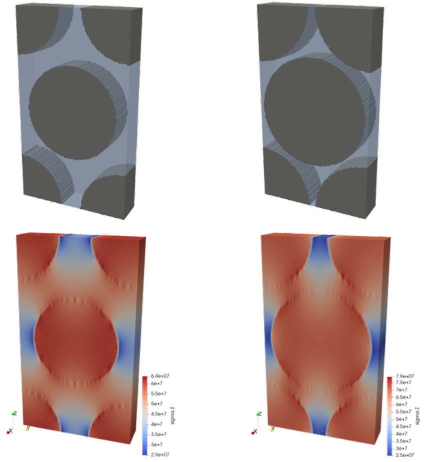
Matrix: porous phenolic resin



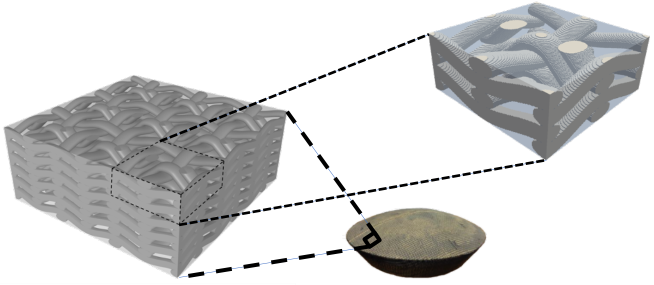


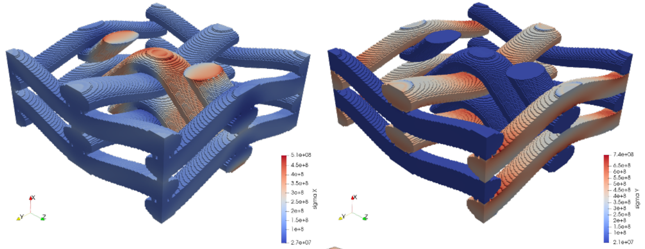
Intra-tow fiber packing

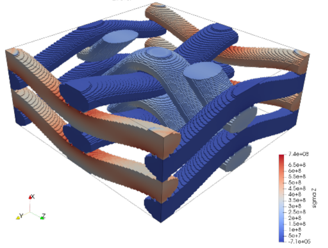




Woven unit cell

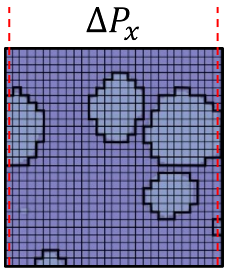




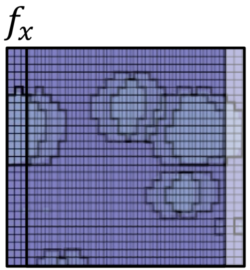


Permeability solver

- Governing equation for Stokes flow (valid for slow creeping regimes, $Re \approx 0$):



$$-\mu\nabla^2\boldsymbol{u} + \nabla p = \boldsymbol{f}$$



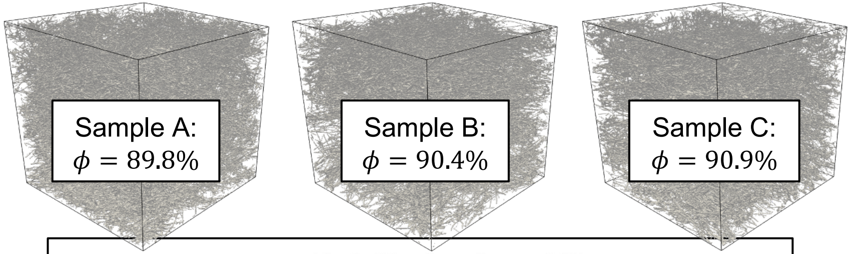
- Solved with FE scheme with Q1-Q1 discretization in velocity and pressure (plus pressure stabilization term)
- By imposing a unit body force f_i in the three Cartesian directions, we can homogenize the permeability as:

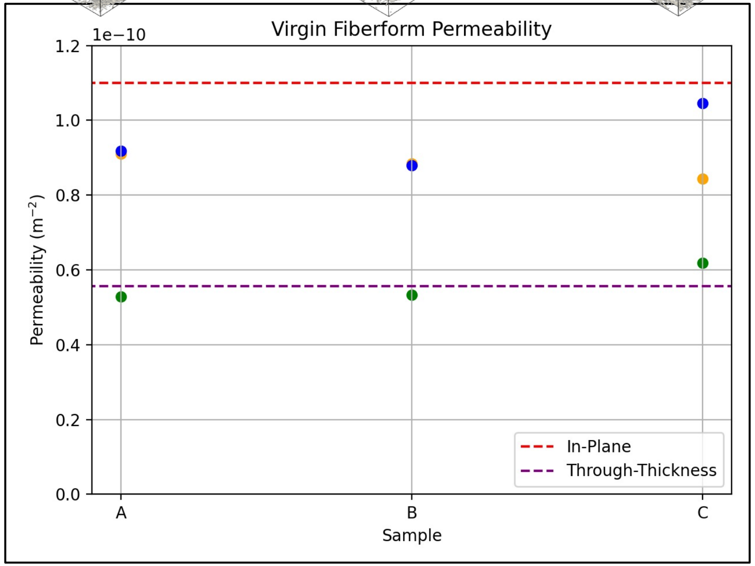
$$\begin{bmatrix} k^{xx} & k^{xy} & k^{xz} \\ k^{xy} & k^{yy} & k^{yz} \\ k^{xz} & k^{yz} & k^{zz} \end{bmatrix} = \frac{l^3}{|V|}\int^{V} u^i \, dV$$

Permeability validation: Fiberform

- Three 500^3 samples with voxel size = 2.6μm
- Run on V100 (32GB) with matrix-free PCG
- Experimental values* obtained from Fiberform samples with porosity $\phi = 87\%$

Sample	A	B	C	Exp*
K_{xx} (m^{-2} e-10)	0.910	0.884	0.845	1.100
K_{yy} (m^{-2} e-10)	0.918	0.879	1.046	1.100
K_{zz} (m^{-2} e-10)	0.529	0.533	0.619	0.557
Porosity ϕ (%)	89.8	90.4	90.9	87.0
Time (') (Avg its)	18.667 (1951)	13.383 (1355)	14.617 (1483)	-
DOFs (e6)	424.4	428.3	432.6	-

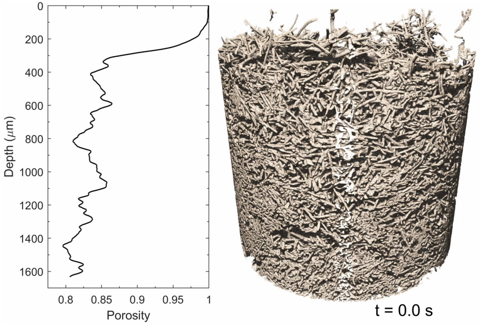




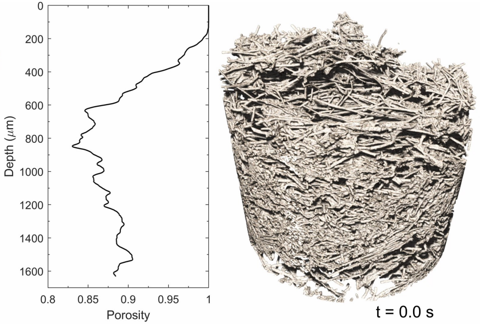
Lopes, P.C.F., Semeraro, F.

*Panerai, F., White, J.D., Cochell, T.J., Schroeder, O.M., Mansour, N.N., Wright, M.J., Martin, A., 2016. Experimental measurements of the permeability of fibrous carbon at high-temperature. *International Journal of Heat and Mass Transfer*, *101*, pp.267-273.

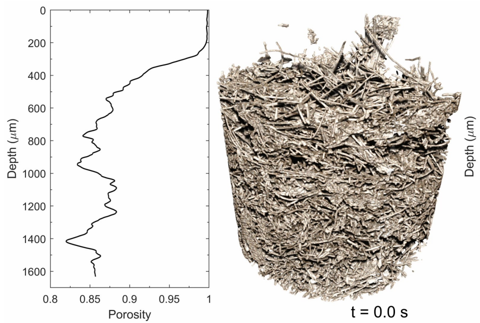
Time-dependent micro-CT of oxidizing Fiberform



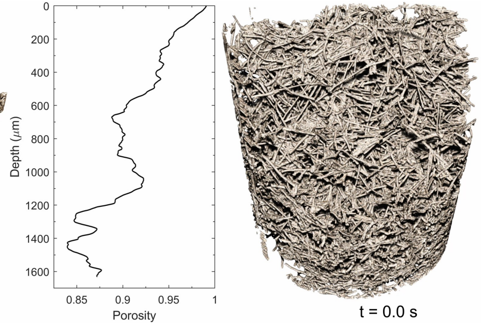
Power	Pressure
13 A	20 torr



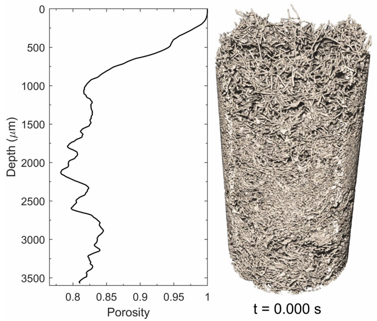
Power	Pressure
13 A	200 torr



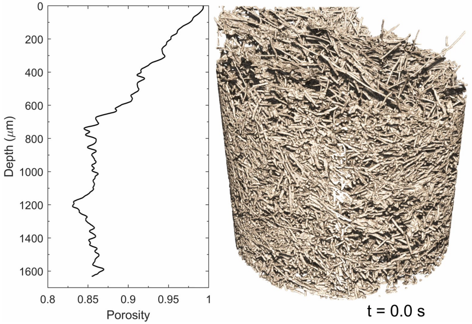
Power	Pressure
15 A	20 torr



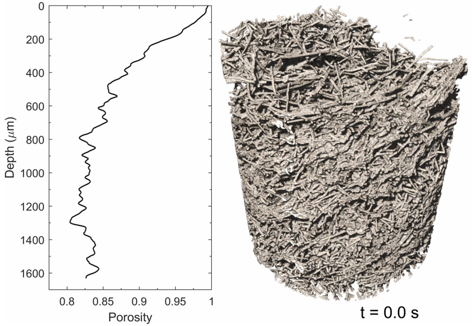
Power	Pressure
15 A	200 torr



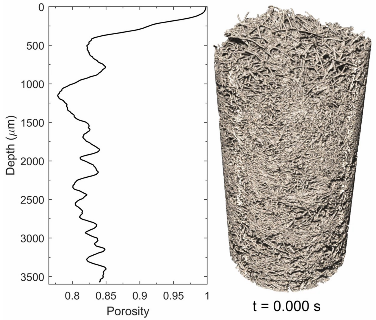
Power	Pressure
15 A	760 torr



Power	Pressure
18 A	20 torr



Power	Pressure
18 A	200 torr



Power	Pressure
19 A	760 torr

Ringel, B., Semeraro, F., Panerai, F.

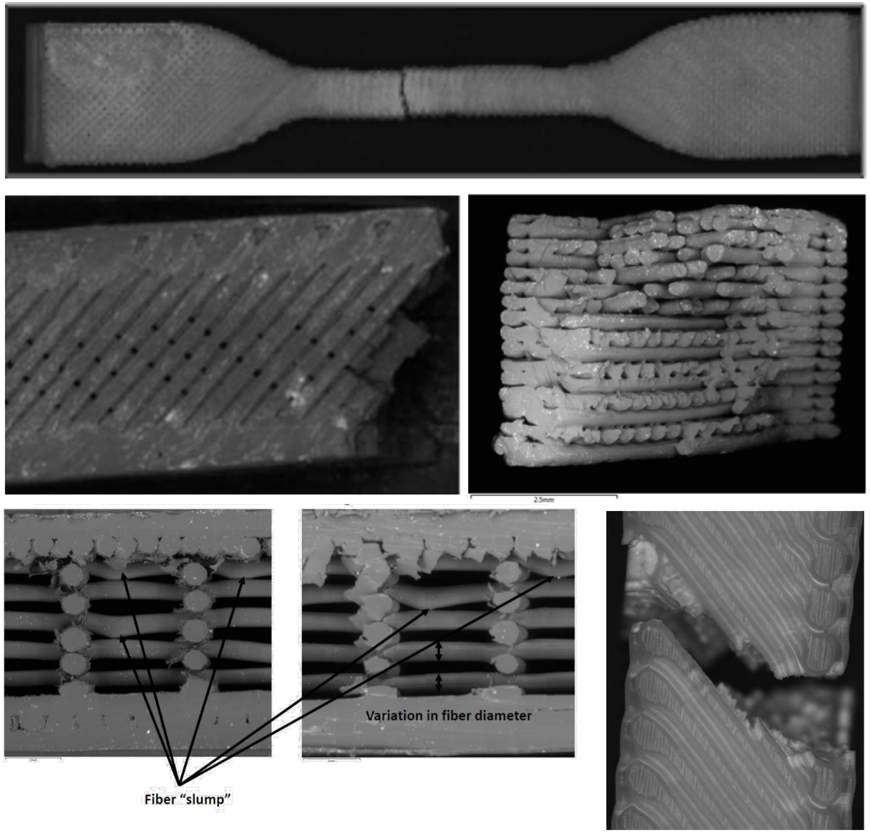
Discussion/questions

https://github.com/nasa/puma

Potential analysis that PuMA could provide:

- Voids/defects/interfaces identification from micro-CT
- Fiber orientation detection and statistics
- Fiber/void segmentation using ML method
- Effective thermo-mechanical properties
- Sensitivity analysis
- Artificial generation from GCODE commands

Tensile test samples from 3DP mission*



*Prater, T., Bean, Q., Werkheiser, N. and Ledbetter, F., 2016, October. 3D Printing in Zero G Technology Demonstration Mission: Summary of On-Orbit Operations, Material Testing and Future Work. In AIAA Young Professionals Symposium (No. M16-5592).